

Tetraethylenepentamine
112-57-2 | DTXSID7026108

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -12.9 °C

Global applicability domain: Outside

Local applicability domain index: 3.29e-01

Confidence level: 3.38e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Tetraethylenepentamine</div> <div>Measured: -30.0</div> <div>Predicted: -12.9</div>	<div>Image not found</div> <div>Triethylenetetramine</div> <div>Measured: 12.0</div> <div>Predicted: 16.4</div>	<div>Image not found</div> <div>1,4-Butanediamine, N,N'-bis(3-aminopropyl)-</div> <div>Measured: 29.0</div> <div>Predicted: 35.0</div>
<div>Image not found</div> <div>Cyclam</div> <div>Measured: 185</div> <div>Predicted: 157</div>	<div>Image not found</div> <div>Pentostatin</div> <div>Measured: 220</div> <div>Predicted: 219</div>	